FG03-89ER13991

Lattice Gas Hydrodynamics - Theory and Simulations Final Report

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Abstract

The first successful application of a microscopic analogy to create a skeleton cellular automaton and analyze it with statistical mechanical tools, was the work of Frisch, Hasslacher and Pomeau on the Navier-Stokes equation in two and three dimensions . This has become a very large research area with lattice gas models and methods being used for both fundamental investigations into the foundations of statistical mechanics and a large number of diverse applications. This present research was devoted to enlarging the fundamental scope of lattice gas models and proved quite successful.

Since the beginning of this proposal, cellular automata have been constructed for statistical mechanical models, fluids, diffusion and shock systems in fundamental investigations. In applied areas, there are now excellent lattice gas models for complex flows through porous media, chemical reaction and combustion dynamics, multiphase flow systems, and fluid mixtures with natural boundaries. With extended cellular fluid models, one can do problems with arbitrary pairwise potentials. Recently, these have been applied to such problems as non-newtonian or polymeric liquids and a mixture of immiscible fluids passing through fractal or spongelike media in two and three dimensions. This proposal has contributed to and enlarged the scope of this work.

Work Accomplished

The original FHP model [16,3] is a model for the simplest fluid, for if any of the fundamental ingredients are removed, one cannot derive the Navier-Stokes equations. In the study of fluids by lattice gas methods, the first aim is extending the range of fluid parameters allowed by a model such as Reynolds number, viscosity and general equations of state. Techniques must be found to suppress the inevitable deviations from true fluid behavior caused by Fermi-Dirac

statistics[11,12]. Even in limited models one can study complex phenomena involving multi-component fluids with interfaces and systems with quite complex boundaries.

There have been many patchwork attempts at lattice gas models in both these directions but recently there has been genuine progress in finding the most fruitful method of enlarging the scope of lattice gas models, useful for both problems.

The FHP model in its original form is a statistical mechanics of hard sphere particles of zero radii and gives an ideal gas law for an equation of state. Effective interactions in the fluid build up by the usual collective motion effects. There is no notion of a fundamental pairwise potential built into the model at a fundamental level since model contains no microscopic transition process[3]. Much more work remains to be done on such generalized schemes which open up lattice gas models to the study of more realistic flows. One should keep in mind that the computational efficiency of lattice gas models in three dimensions increases as the fourth power of the Reynolds coefficient, so significantly improving that number implies a rapid gain in simulation power.

Clearly, such primitive models are a first step. The problem is particularly acute in three dimensions, and we have designed experimental three dimensional lattice gas fluid models with as few as sixteen bits as well as working on optimizing lookup table access for the standard twenty-six bit model by simulated annealing techniques on rule space to find the smallest number of equivalence classes of rules.

Multicomponent Models and Models with Complex Boundaries.

The other kinds of systems that are exceptionally well modeled by even ordinary lattice gases are variations on two phase immiscible fluid flow with an interface. One can study this alone or add to it complex boundaries made of porous structures, which is especially valuable for three dimensional studies of flow through porous media. These models extend the range of phenomena lattice fluids can simulate and mathematically model to porous media, froths, minimal surface problems, fingering phenomena and general two fluid instabilities, leading to a study of the dynamics of fluid mixtures. In many cases, these phenomena were accessible before this only by experiment.

The simplest two phase immiscible fluid model with surface interfaces is a contracted version of the extended neighborhood model discussed above [19].

In outline, one introduces two copies of the FHP hexagonal gas in two dimensions and makes them distinguishable by introducing tags say red and blue colors. In each phase separately, we have the usual incompressible Navier-Stokes equations. The colored fluids now couple only through interface boundary conditions; that the normal component of interface velocity equals the component of velocity locally normal to the boundary and that the stress difference at the interface is equal to the surface tension

These are implemented by introducing a flux of colored particles and a color field which is the weighted sum of the difference between red and blue particles at neighboring sites. One now asks that the work done against the color field by the color flux be a minimum. Such a model preserves color mass separately and has total momentum conservation. This usually defines an equivalence class of solutions to the minimization problem and collisions are chosen from this class with equal weight. This simple model describes the interface dynamics of a two fluid immiscible system very well and is computationally efficient [19].

There is considerable evidence [21] that such a model accurately captures the puzzling features of pattern formation in the early stages of Ragleigh-Bernard convection in which one looks at stochastic effects on the system near the convective onset an observation which should be further explored.

These models need considerable development and we intend to do so since the range of complex phenomenon they simulate is both large and important. Recent experimental runs with porous media boundary conditions taken from actual porous rock samples show agreement with experimental measurements on pressure profiles to within a few percent.

Lattice Gases Which Dynamically Alter the Geometry of the Lattice.

A central issue in cellular automata formulations of physical systems is whether they can ever capture the dynamics of systems which have no natural collision model underlying the physics. Additionally many physical systems have some version of gauge invariance built into them. Plasmas, for example, contain the Maxwell equations as an integral part of their dynamics and we must deal with the electromagnetic sector of these models in an accurate way.

The example above of the extended neighborhood lattice gas had new cellular automata sites capable of fission and fusion with some probability [36]. Imagine this lattice gas automaton as a two layered gas, a layer containing indivisible particles scattering as in the original hexagonal FHP model, and a layer

containing only the new species of active particles.

One considers this layer of active particles as defining the vertices of a triangulation and takes the dual graph so that points go to faces and faces to vertices in the usual way. Then the annihilation and creation of active particles goes over to the creation and destruction of edges in the dual graph which has a dynamics given by the original gas rules. This is a special example of a new class of general lattice gases which dynamically alter the geometry of the spaces on which they were originally defined. There are applications to fields as diverse as field theory , computational geometry, image processing and random surface theory.

This is a class of novel lattice gases which will be important to our understanding of cellular automata in general and may have many applications to mathematics, physics and computer science. Fundamental and applied studies of various cellular automata are usually done on a lattice of fixed geometry. This includes all of the discrete models that simulate field theories ordinarily described by partial differential equations. There are two reasons for this: The first is simplicity - fixed lattices are simple to work on; the second is that lattice topology is usually assumed to decouple from the dynamics of discrete systems. Dynamics is thought of as contained in the evolution of site variables that occupy the lattice and in these alone. This is unsatisfactory for many reasons:

Intuitively, physics uses lattices which are closer to randomly arranged than regular. Since we are unable to explore random lattices directly, a cellular automaton that develops a random structure can smoothly take us to that regime. Regular lattice arrangements also produce shadows of themselves - their symmetry appears in the macroscopic field theory either if one is not careful to adjust the automaton to wash it out or if the correlations length on the lattice is finite [3,11].

On fixed lattices, dynamical models where a collision process is the fundamental one, naturally split up into two distinct operations: Free streaming to vertices, and then a collision. The transcription of collision dominated models as a one step cellular automaton forms an automaton with a large neighborhood. These are quite difficult to study [42]. Both the Navier-Stokes automaton and dynamic Ising-like models are examples.

A new class of automata emerges if one allows the geometry of the lattice to be dynamical, in the sense of a dynamical variable [43]. Then we have a generalized automaton, which one might think of as a dynamical triangulation of a manifold coupled to spin matter [44]. The most general case has no predetermined idea of an embedding manifold or of triangulation.

This is class of lattice gases where site values and links between points are treated with equal weight. One can move from a bit description to a link description indifferently. In this way, we have a duality between state variables and the geometry of the lattice. By studying the possible classes of lattice gases, whose evolution modifies the automaton connectivity in a self-consistent way, one encounters extraordinary new mathematical objects. Topological lattice gases consist of site updating in the usual sense of cellular automata, and operations which annihilate and create links, according to lists of updating rules.

Dimension is a topological invariant, which means it cannot change under continuous evolution. Topological lattice gases, are not continuous so one can have automata which build up dimensionality, in the Hausdorff scaling sense, as part of their dynamics. This behavior has been observed in classes of these objects [45,5]. When dimensionality becomes stable over a certain length scale, topological lattice gases dynamically generate a fundamental length, as that distance over which an effective dimension has acceptable fluctuations. By choosing other scaling quantities, various fundamental length scales can be introduced into a model in a purely dynamical way. This is a powerful mechanism, useful in many problems.

Topological lattice gases open a new degree of freedom in discrete dynamics. The closest analog to such systems is the Regge calculus formulation of classical general relativity [46,47] where matter and a simplex description of a manifold are coupled and lead self-consistently to the classical Einstein equations [48]. Those are more complex systems than usually studied, but which may be functionally simpler - there is more room for fixed point equations and adjustable parameters.

The applications for these systems are important: Self-adjusting grids and site rules which are faithful to dynamics, simulation of complex self-organizing behavior of every kind and new algorithmic attacks on complex systems. In a physical setting, these models are ideal for any theory described by a fiber bundle structure with a connection. This includes all the general gauge models - Maxwell, Yang-Mills, classical and quantum gravity, plasmas and extended objects such as field theories built of random strings and surfaces [49,50,53]. This idea has already been explored to create totally discrete models for two dimensional quantum gravity. It produces the same results as quite sophisticated continuum quantum field theory techniques . By using these topological cellular automata ideas we were able to see an order of magnitude speedup in convergence of simplex grid problems ordinarily done by Metropolis techniques.[51].

Collision dominated automata, which are discrete field theory models for many complex systems, in the world of ordinary length scales and energies of a few electron volts, can be written as cell complex automata with small neigh-

borhoods. We found that it is quite possible that by dynamically changing the topology of the space as the automaton evolves, unusually compact and efficient computational algorithms will be found for many nonlinear extended systems [52].

Finally, topological lattice gases have a great deal to teach about new ways to organize the architecture of parallel computers, whether they are physical or virtual architectures. These automata are potentially very rich structures and we propose to study them both by analytic methods and computer simulations.

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